Amendments to the Abstract

Please delete the Abstract and add the following new Abstract:

A method of analysing on a computer 2-dimensional or 3-dimensional chemical data is disclosed together with a computer program product for the same. The method includes the steps of: a) cluster analysis on the data using a distance metric for the distance between point x and point y of the form:

$$D(x,y) = 4\sin^2\left(\frac{\alpha}{2}\right) + \frac{(r_x - r_y)^2}{r_x r_y}$$

where α is the angle between point x and point y and r_x and r_y are, respectively, the distances from the co-ordinate origin to point x and point y; and b) outputting the results of the cluster analysis from the computer.